New Low Thermal Conductivity Materials for Thermoelectric Applications

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A low lattice thermal conductivity is one of the conditions required to achieve high thermoelectric figures of merit. Several low thermal conductivity materials were identified and developed over the past few years at JPL, including filled skutterudites and Zn_4Sb_3-based materials. A study of the mechanisms responsible for the high phonon scattering rates in these compounds has demonstrated that materials with highly disordered structures or complex structures which can accommodate additional atoms in their lattice are likely to have low lattice thermal conductivity. Chevrel phases based on Mo_6Se_8 are just such materials and are currently being investigated at JPL. The crystal structures of the Chevrel phases present cavities which can greatly vary in size and contain a large variety of atoms ranging from large ones such as Pb to small ones such as Cu. These atoms are not localized in the structure and, depending on their size, can move between different sites. We believe that they can produce significant phonon scattering and result in low lattice thermal conductivity. Although most of the Chevrel phases studied until now were reported to be metallic, it was found that semiconducting Chevrel phases can be created by controlling the number of electrons per $[Mo_6]$ cluster. Initial results obtained on the thermoelectric properties of semiconducting Chevrel phases are presented. Various approaches to determine the potential of this large family of compounds (over 100 are known) for thermoelectric applications are discussed.

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